# National Center for Computational Sciences Snapshot
# The Week of December 17, 2007

**Researchers at ORNL Solving Mysteries behind Biomolecules**
*Simulations show potential in medicine, energy*

Proteins are highly efficient biological machines, but some "tinkering" could make them better.

That conviction drives the use of scientific simulation to provide a more detailed understanding of how biomolecules such as proteins and enzymes operate. (An enzyme is a type of protein that catalyzes or speeds up a chemical reaction.) Ultimately, the research, conducted on the National Center for Computational Sciences (NCCS) Jaguar supercomputer, is expected to pave the way for designing enzymes that operate more efficiently and harnessing them to improve the efficiency of chemical processes.

"The implications of the fundamental understanding of biomolecular systems will be felt in many fields, including health and medicine, energy, and the environment," said Pratul Agarwal of Oak Ridge National Laboratory (ORNL), principal investigator for the project.

The pioneering biomolecular simulations have produced major new insights into protein structure, dynamics, and functions. A focus of Agarwal's research was the internal dynamics of the cellulase enzyme, which converts the cellulose in biomass into sugars. "Once we understand the mechanism of this enzyme, we will be able to design better or more efficient enzymes so we can improve the process for producing ethanol at low cost," Agarwal said.

Cellulase function involves two different activities of interest. First, Agarwal explained, the enzyme binds to the cellulose surface and splits off individual cellulose chains, which involves breaking hydrogen bonds. Second, linkages in the cellulose chains are hydrolyzed to release glucose or slightly more complex sugar units, which can be converted to ethanol. Releasing sugars from the cellulose chains is what currently limits the efficiency and cost-effectiveness of ethanol production. More efficient cellulases are needed. Once the mechanisms for splitting off cellulose chains and for releasing sugars are understood, Agarwal said, scientists will have an idea of the amino acids that can be optimized through protein engineering for more efficient conversion of cellulose to sugar.

Another enzyme being investigated is cyclophilin A (CyPA), a protein of medical interest because it plays a role in HIV-1 infection. Understanding the mechanism of CyPA functioning and its role in the HIV-1 life cycle could guide researchers in finding a way to slow the spread of the AIDS virus. CyPA also influences protein folding (the process by which a chain of amino acids folds into a three-dimensional protein structure). Correct folding is essential for proteins to function properly, and misfolded proteins cause disorders such as Alzheimer's disease and brain-wasting illnesses.

"The power of computational techniques such as the ones we are using is that they provide a very good collective set of information on a variety of time and length scales. So we get a very complete picture from computational studies."

"These simulations on NCCS resources allowed us to investigate multiple proteins from different species simultaneously to provide new insights," he said.

## ORNL Hosts Computational Materials Workshop

*Buongiorno Nardelli addresses the finer points of simulation*

The success of nanotechnology is becoming increasingly dependent on the ability of scientists to computationally model the properties of various materials and nanostructures. As a result, today's nanoscientists rely more and more on the art of simulation to successfully integrate theory, experiment, and modeling.

To address this growing demand, Dr. Marco Buongiorno Nardelli, an associate professor of physics at North Carolina State University with a joint appointment with the Computer Science and Mathematics Division at ORNL, held a "Computational Materials Workshop" at ORNL December 10–14.

The lectures, which were based on the latest research in nanoscale physics and engineering, were supplemented with hands-on exercises and simulations using the state-of-the-art software suite "quantum-ESPRESSO."

"The workshop was very successful," said Nardelli, adding that on average 10–15 people were attending at any one time. "It was a lot of work, but I am very pleased overall." Nardelli said that next time around he plans to have multiple guest lecturers. "I think it will become something regular," he said, adding that he thinks the workshop could be conducted once every one and a half to two years.

Topics covered included basic algorithms and functionalities for electronic structure simulations of materials, lattice dynamics, and statistical mechanics and molecular dynamics.

## ORNL Attends TeraGrid Workshop

*National Science Foundation prepares for petascale at Arizona State University*

A contingent from ORNL attended and participated in a petascale preparation workshop held December 11–12 at Arizona State University's Fulton School of Engineering.

The workshop, titled "Building PetaScale Applications and Software Environments on TeraGrid," featured a series of lectures and presentations on algorithms, techniques, and performance tools.

Ricky Kendall, group leader for the scientific computing group at the NCCS and acting group leader for the National Institute for Computational Sciences (NICS), discussed the new NICS facility at ORNL. Bronson Messer of ORNL presented information on parallel compilers and languages.

NICS was established as the result of a recent National Science Foundation grant. It will house a new near-petascale computer fully integrated with TeraGrid, giving the state of Tennessee two of the nation's fastest supercomputers.

"Petascale application developers and petascale tool developers had the opportunity to get together and share expectations, plans, and needs," said Don Frederick, an attendee and member of the User Assistance and Outreach Group at the NCCS. "The key will be the follow-up," he added, alluding to the group's future interactions.

**ORNL Hosts CPES Workshop**

*Scientists present latest breakthroughs in plasma edge research*

Members of the Center for Plasma Edge Simulation (CPES) met December 3 and 4 at ORNL for a comprehensive workshop on the team's efforts.

The team, headed by C.S. Chang of New York University, is steadily uncovering the mysteries surrounding plasma edge research, a particularly vexing field of fusion science.

According to team member Scott Klasky of ORNL, CPES is developing "state-of-the-art first principles codes that look at the effects on the edge of the plasma," adding that edge simulation is a popular issue in fusion research.

Klasky discussed two codes in particular. The first, XGC0, is a neoclassical particle code that doesn't look specifically at plasma turbulence but does examine many of the kinetic effects that happen at the edge of a plasma.

The second, XGC1, is also a neoclassical code that sheds light on both kinetic effects and turbulence self-consistency at the plasma edge. XGC1 has run on 16,000 processors and, according to Klasky, has shown "fantastic results." The code, he adds, "is a good mixture of applied mathematics, physics, and computer science."

Also on display were the latest breakthroughs from the team's researchers, who came from across the nation to attend the workshop. In particular, a tutorial on the user-friendly Kepler workflow engine "added excitement," said Chang. The new data arrangement and archiving system enables scientists to concentrate on the work in their fields and not worry about the technical portion of simulation. Physicists can talk physics, leaving the computer science to computer scientists, said Klasky.

Other highlights of the workshop included the first computational understanding of the Resonance Magnetic Perturbation experiment and new deterministic collision operators.

The workshop was held at the Joint Institute for Computational Sciences building at ORNL.

## Seminar Series Investigates New HPC Platform

*Exploring LANL'S Roadrunner at ORNL*

ORNL recently hosted a seminar entitled "Early Experiences in Hybrid Computing" about a new high-performance computing platform at Los Alamos National Laboratory (LANL).

The seminar, held November 27 as part of the National Center for Computational Sciences Seminar Series, was conducted by John A. Turner, group leader for the computational physics group at LANL.

Turner outlined "early experiences and results" of science applications on the new LANL platform, known as Roadrunner. According to Turner, Roadrunner "will consist of a relatively-standard cluster of general-purpose commodity AMD Opteron processors augmented by high-performance hardware accelerators based on the Cell Broadband Engine used in the Sony Playstation 3 video game console."

Although the machine will likely achieve petascale performance on various benchmarks such as LINPACK, tailoring relevant scientific applications to the new platform could prove to be a challenge.

According to Turner, "success will require both the development of software tools and a rethinking of current algorithmic and code development approaches and practices."